

6-methyl-nonacosane

Other names:	Nonacosane, 6-methyl
Inchi:	InChI=1S/C30H62/c1-4-6-8-9-10-11-12-13-14-15-16-17-18-19-20-21-22-23-24-25-27-29
InchiKey:	QJJWGHQCDHJHSX-UHFFFAOYSA-N
Formula:	C30H62
SMILES:	CCCCCCCCCCCCCCCCCCCCCCCC(C)CCCC
Mol. weight [g/mol]:	422.81

Physical Properties

Property code	Value	Unit	Source
gf	199.28	kJ/mol	Joback Method
hf	-667.81	kJ/mol	Joback Method
hfus	69.93	kJ/mol	Joback Method
hvap	81.99	kJ/mol	Joback Method
log10ws	-12.14		Crippen Method
logp	11.805		Crippen Method
mvol	433.560	ml/mol	McGowan Method
pc	597.80	kPa	Joback Method
rinpol	2950.00		NIST Webbook
rinpol	2948.10		NIST Webbook
tb	885.36	K	Joback Method
tc	1090.03	K	Joback Method
tf	412.86	K	Joback Method
vc	1.710	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1482.38	J/molxK	885.36	Joback Method
cpg	1509.50	J/molxK	919.47	Joback Method
cpg	1535.09	J/molxK	953.58	Joback Method
cpg	1559.23	J/molxK	987.69	Joback Method
cpg	1582.00	J/molxK	1021.80	Joback Method
cpg	1603.48	J/molxK	1055.92	Joback Method
cpg	1623.76	J/molxK	1090.03	Joback Method

dvisc	0.0013422	Paxs	412.86	Joback Method
dvisc	0.0003919	Paxs	491.61	Joback Method
dvisc	0.0001607	Paxs	570.36	Joback Method
dvisc	0.0000818	Paxs	649.11	Joback Method
dvisc	0.0000482	Paxs	727.86	Joback Method
dvisc	0.0000315	Paxs	806.61	Joback Method
dvisc	0.0000222	Paxs	885.36	Joback Method

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R418130&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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